AMENDMENTS TO THE CLAIMS

1. (CURRENTLY AMENDED) A computer-implemented method of predicting functional similarity between two molecules comprising:

deriving a first one-dimensional representation of a first molecule from distances between selected atoms of said first molecule, wherein the selected atoms of the first molecule are assigned positions in the first one-dimensional representation;

deriving a second one-dimensional representation of a second molecule from distances between selected atoms of said second molecule, wherein the selected atoms of the second molecule are assigned positions in the second one-dimensional representation; and

comparing said one dimensional representations.

2. (ORIGINAL) The method of Claim 1, wherein said one-dimensional representations comprise linear representations.

3. (ORIGINAL) The method of Claim 2, wherein said deriving comprises calculating a linear position for each of a plurality of selected atoms of said first molecule.

4. (ORIGINAL) The method of Claim 3, wherein said linear positions are selected to reduce the deviation between relative positions of said plurality of selected atoms along a line and three dimensional distances between said plurality of atoms in said first molecule.

5. (ORIGINAL) The method of Claim 3, wherein said deriving comprises calculating a linear position for each of a plurality of selected atoms of said second molecule.

6. (ORIGINAL) The method of Claim 5, wherein said comparing comprises aligning said one dimensional representations so as to match linear positions of at least one of said selected atoms of said first molecule with at least one of said selected atoms of said second molecule.

7. (ORIGINAL) The method of Claim 6, wherein said matched atoms have the same element type.

8. (ORIGINAL) The method of Claim 7, wherein said matched atoms have the same hybridization state.

9. (ORIGINAL) The method of Claim 1, wherein at least some of said distances are derived from molecular topology.

10. (ORIGINAL) The method of Claim 9, wherein at least some of said distances are derived from bond counts.

11. (ORIGINAL) The method of Claim 1, wherein at least some of said distances are derived from three dimensional atomic coordinates.

12. (ORIGINAL) A computer implemented method of comparing molecules comprising:

representing a first molecule as a first set of selected atoms, wherein each atom of said first set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms;

representing a second molecule as a second set of selected atoms, wherein each atom of said second set is associated with an atom type and a scalar value, wherein the scalar values are derived from distances between said selected atoms; and

comparing said atom types and scalar values.

13. (ORIGINAL) The method of Claim 12, wherein said scalar value represents a linear position.

14. (ORIGINAL) The method of Claim 13, wherein each atom of said set is associated with a second scalar value, said second scalar value representing a width centered about each of said linear positions.

15. (ORIGINAL) The method of Claim 13, wherein said comparing comprises:

aligning the linear positions of an atom in the first molecule with an atom of the same type in the second molecule such that their lengths completely overlap; and

evaluating the amount of overlap between atoms of the first molecule and atoms of the same type of the second molecule.

16. (ORIGINAL) The method of Claim 15, comprising repeating the aligning and evaluating steps so as to evaluate the overlap at all linearly aligned positions of atom pairs having the same type.

17. (ORIGINAL) The method of Claim 14, wherein said second scalar value is the same for all of said selected atoms.

18. (CURRENTLY AMENDED) A computer-implemented method of representing a non-linear three dimensional configuration of a molecule made up of a plurality of bonded atoms, said method comprising assigning, to at least some of said atoms, a position along a line so as to define a set of linear distances between each of said selected atoms, wherein at least some of said linear distances are not equal to the corresponding three dimensional distances between the same atoms in said molecule.

19. (ORIGINAL) The method of Claim 18 comprising reducing a total deviation between said set of linear distances and the corresponding three dimensional distances between the same atoms in said molecule.

20. (CURRENTLY AMENDED) A computer-implemented method of representing a non-linear three dimensional configuration of a molecule made up of a plurality of bonded atoms, said method comprising assigning, to at least some of said atoms, a position along a line so as to define a set of linear distances between each of said selected atoms, wherein at least some of said linear distances are not equal to corresponding topologically defined distances between the same atoms in said molecule.

21. (ORIGINAL) The method of Claim 20 comprising reducing a total deviation between said set of linear distances and the corresponding topological distances between the same atoms in said molecule.

22. (CURRENTLY AMENDED) A computer-implemented method of selecting for further testing and analysis a subset of molecules from a library of molecular structures, said method comprising:

storing linear representations of said molecular structures in a database, said linear representations being derived from three dimensional distances or topological distances between atoms of said molecular structures, wherein at least some of the atoms of each molecular structure are assigned positions in the respective linear representations;

deriving a linear representation of a molecule having known biochemical activity from three dimensional distances or topological distances between atoms of said molecule; wherein at least some of the atoms of said molecule are assigned positions in the respective linear representations;

comparing said linear representation of said molecule having known biochemical activity with said linear representations of said molecular structures in said database.

23. (CURRENTLY AMENDED) A computer-implemented method of molecular parameterization comprising:

selecting a set of atoms in said molecule;

deriving a set of scalar values from distances between said selected atoms;

assigning to each of said selected atoms a parameter set including an atom type and one of said set of scalar values.

24. (ORIGINAL) The method of Claim 23, wherein said set of scalar values represents a set of linear positions.

25. (ORIGINAL) The method of Claim 24, additionally comprising assigning a second scalar value to each of said selected atoms, said second scalar value representing a width centered about each of said linear positions.

26. (ORIGINAL) The method of Claim 25, wherein said second scalar value is the same for all of said selected atoms.

27. (ORIGINAL) The method of Claim 23, wherein said distances comprise three dimensional distances.

28. (ORIGINAL) The method of Claim 23, wherein said distances comprise topological distances.

29. (ORIGINAL) A method of drug discovery comprising comparing molecules that have been parameterized according to the method of Claim 23.

30. (ORIGINAL) A computer readable storage medium having stored thereon structural representations of molecules for retrieval by a computer implemented molecular screening program, wherein at least one of said structural representations comprises a list of selected atoms in said molecule, wherein each of said selected atoms is associated with an atom type and a scalar value.

31. (ORIGINAL) The method of Claim 30, wherein said scalar value is derived from distances between said selected atoms in said molecule.

32. (ORIGINAL) The method of Claim 31, wherein said distances comprise three dimensional distances.

33. (ORIGINAL) The method of Claim 31, wherein said distances comprise topological distances.

34. (ORIGINAL) The computer readable storage medium of Claim 30, wherein said scalar value comprises a position in a linear representation of said molecule.

35. (CURRENTLY AMENDED) A computer implemented method of predicting one or more chemical properties of a molecule comprising:

retrieving a linear representation of a first molecule having a known chemical property, said linear representation comprising a set of atoms and associated linear positions in the linear representation of the first molecule;

retrieving a linear representation of a second molecule, said linear representation comprising a set of atoms and associated linear positions in the linear representation of the second molecule; and

comparing said linear representations.